



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:27 PM GMT

PDB ID : 1AR8
Title : P1/MAHONEY POLIOVIRUS, MUTANT P1095S
Authors : Wien, M.W.; Curry, S.; Filman, D.J.; Hogle, J.M.
Deposited on : 1997-08-11
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

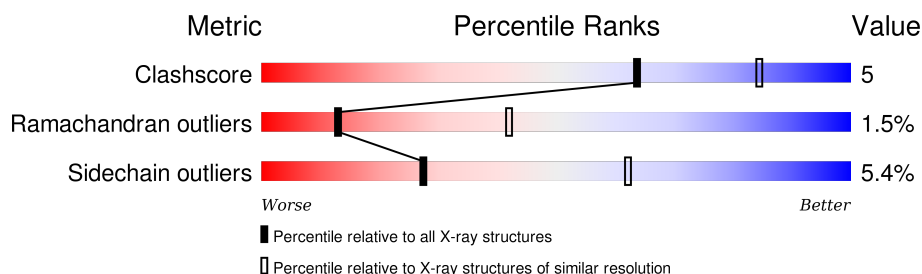
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	8	<div> <div>25%</div> <div>75%</div> </div>
2	1	302	<div> <div>77%</div> <div>15%</div> <div>6%</div> </div>
3	2	272	<div> <div>79%</div> <div>16%</div> <div>5%</div> </div>
4	3	238	<div> <div>84%</div> <div>13%</div> <div>3%</div> </div>
5	4	68	<div> <div>66%</div> <div>18%</div> <div>12%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7184 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	0	8	Total	C	N	O	0	0	0
			43	24	8	11			

- Molecule 2 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	283	Total	C	N	O	S	0	0	0
			2221	1414	378	424	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	95	SER	PRO	ENGINEERED	UNP P03300

- Molecule 3 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	268	Total	C	N	O	S	0	0	0
			2085	1317	358	396	14			

- Molecule 4 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	235	Total	C	N	O	S	0	0	0
			1834	1169	299	349	17			

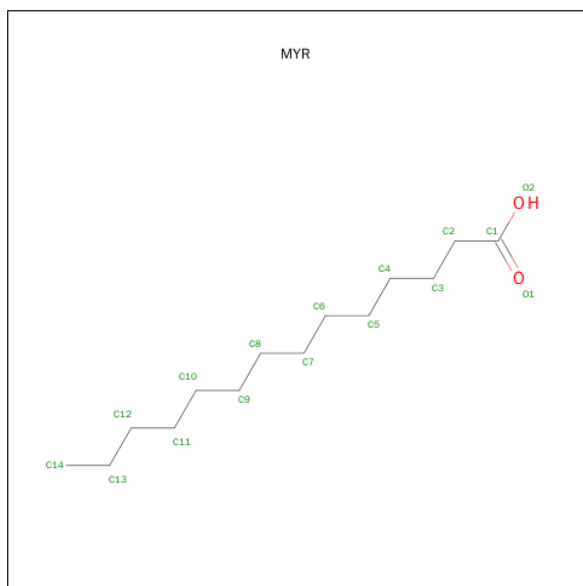
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	CONFLICT	UNP P03300

- Molecule 5 is a protein called P1/MAHONEY POLIOVIRUS.

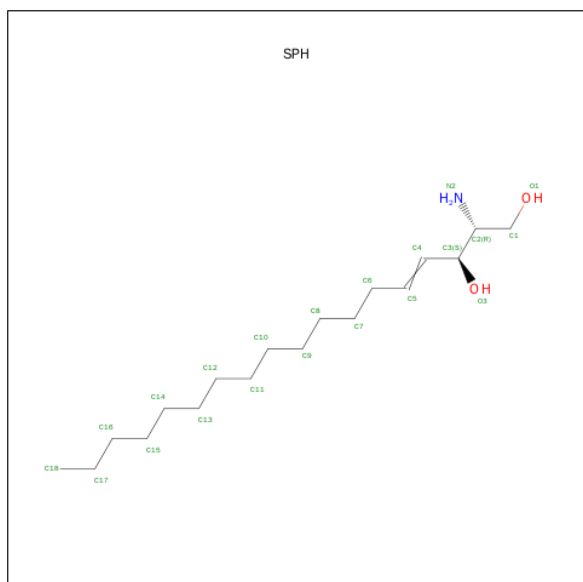
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	60	Total	C	N	O	S	0	0	0
			462	286	78	97	1			

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	4	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	1	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	0	1	Total	O	0	0
			1	1		
8	1	184	Total	O	0	0
			184	184		
8	2	143	Total	O	0	0
			143	143		
8	3	135	Total	O	0	0
			135	135		
8	4	40	Total	O	0	0
			40	40		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: P1/MAHONEY POLIOVIRUS

Chain 0: 

A3
A4
A5
A6
S7
S8
S9
T10


• Molecule 2: P1/MAHONEY POLIOVIRUS

Chain 1: 

GLY
LEU
GLN
GLN
MET
LEU
GLU
SER
MET
ILE
ASP
ASN
THR
VAL
ARG
GLU
THR
VAL
GLY
L20
R24
L27
P28
P40
P48
P48
P64
R83
I89
N94
S95
A96
S97
T98
T99
V107
V108
K109
V116
R129
T145
N146
N147
G148
H149
M158
Y159

W170
W176
W176
T177
N180
P181
S182
P191
V196
S206
K218
D219
Q220
S221
A222
D226
S233
L234
D236
F237
G238
I239
H248
K252
R258
K264
W269
P273
K287
L294
S295
T296
Y302


• Molecule 3: P1/MAHONEY POLIOVIRUS

Chain 2: 

SER
PRO
ASN
ILE
E5
C7
G8
Y9
S10
D11
R12
V13
Q26
N30
A34
R37
W38
S45
M48
P49
Q52
A60
F63
W71
T72
K73
W78
W79
W80
A114
P128
N137
T138
T139
T143
Q146
P150
G151
E152
T158

M165
M166
T167
T168
R173
Y179
L187
G188
M189
I197
P211
Y212
V213
W227
F239
L240
S241
P242
S243
L251
A254
P255
R264
R270
L271
Q272

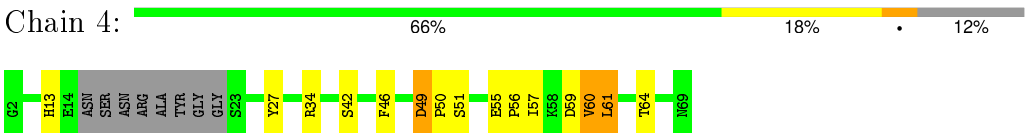
• Molecule 4: P1/MAHONEY POLIOVIRUS

Chain 3: 

G1
Y13
P33
P37
F55
D56
L57
T64
M68
E66
M67
R71
L85
S86
L87
S88
S91
W110
M124
K143
K146
M149
L150
W156
S163
V167
V168
P169
W170
Y189
I190
R206
E207
M208
G212
N218
L224
L225
R226

Q233
R234
L235
LEU
ALA
GLN

• Molecule 5: P1/MAHONEY POLIOVIRUS



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	323.04Å 358.22Å 380.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.00 – 2.90	Depositor
% Data completeness (in resolution range)	34.0 (11.00-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.270 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7184	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPH, MYR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.47	0/41	1.53	0/53
2	1	0.81	0/2283	1.36	23/3120 (0.7%)
3	2	0.84	1/2142 (0.0%)	1.43	20/2928 (0.7%)
4	3	0.79	0/1881	1.28	12/2562 (0.5%)
5	4	0.75	0/469	1.37	3/632 (0.5%)
All	All	0.81	1/6816 (0.0%)	1.36	58/9295 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	7	CYS	CB-SG	5.06	1.90	1.82

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	5	GLU	OE1-CD-OE2	-10.41	110.80	123.30
3	2	78	TRP	CD1-CG-CD2	8.50	113.10	106.30
2	1	175	TRP	CD1-CG-CD2	8.48	113.08	106.30
2	1	170	TRP	CD1-CG-CD2	8.36	112.99	106.30
4	3	110	TRP	CD1-CG-CD2	8.33	112.96	106.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	43	0	39	2	0
2	1	2221	0	2171	29	0
3	2	2085	0	2000	27	0
4	3	1834	0	1816	18	0
5	4	462	0	446	7	0
6	4	15	0	27	1	0
7	1	21	0	37	4	0
8	0	1	0	0	0	0
8	1	184	0	0	3	0
8	2	143	0	0	2	0
8	3	135	0	0	2	0
8	4	40	0	0	0	0
All	All	7184	0	6536	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 69 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:158:MET:SD	2:1:177:THR:HG23	2.16	0.85
3:2:5:GLU:OE2	3:2:7:CYS:HB3	1.78	0.83
4:3:124:MET:HG3	8:3:277:HOH:O	1.81	0.80
1:0:6:ALA:CA	1:0:7:SER:N	2.48	0.76
2:1:177:THR:HG22	2:1:180:ASN:HB2	1.69	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	4/8 (50%)	3 (75%)	0	1 (25%)	0	0
2	1	281/302 (93%)	256 (91%)	21 (8%)	4 (1%)	14	44
3	2	266/272 (98%)	246 (92%)	15 (6%)	5 (2%)	10	35
4	3	233/238 (98%)	222 (95%)	10 (4%)	1 (0%)	39	74
5	4	56/68 (82%)	51 (91%)	3 (5%)	2 (4%)	4	18
All	All	840/888 (95%)	778 (93%)	49 (6%)	13 (2%)	13	42

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	99	THR
3	2	166	ASN
1	0	4	ALA
2	1	147	ASN
2	1	234	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	1	245/261 (94%)	235 (96%)	10 (4%)	37	73
3	2	228/232 (98%)	213 (93%)	15 (7%)	21	51
4	3	210/212 (99%)	201 (96%)	9 (4%)	35	71
5	4	52/57 (91%)	48 (92%)	4 (8%)	16	42
All	All	739/766 (96%)	699 (95%)	40 (5%)	27	62

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	139	THR
3	2	165	ASN
5	4	42	SER

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Mol	Chain	Res	Type
3	2	152	GLU
3	2	168	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	2	165	ASN
5	4	31	ASN
4	3	218	ASN
3	2	48	ASN
5	4	13	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	SPH	1	0	-	19,20,20	0.42	0	16,21,21	1.98	3 (18%)
6	MYR	4	1	5	14,14,15	0.49	0	12,13,15	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SPH	1	0	-	-	0/21/21/21	0/0/0/0
6	MYR	4	1	5	-	0/11/12/13	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1	0	SPH	O3-C3-C2	-4.80	99.47	107.48
7	1	0	SPH	O3-C3-C4	-4.40	98.42	110.78
7	1	0	SPH	O1-C1-C2	3.35	118.57	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1	0	SPH	4	0
6	4	1	MYR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.